

Application of Thermodynamics to the Reduction of Data Generated by a Non-Standard System

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1 Introduction

The purpose of this paper is to illustrate the application of thermodynamics as a pedagogy for the organization, dimensional reduction and analysis of data. To accomplish this it is necessary to build a bridge between the world of everyday experience (a sequence of events occurring in time) and the more abstract world of constant energy surfaces, microcanonical distributions and the notions of work and heat.

Both worlds meet at the path, although an experimentalist may speak of it in terms of observations contained in a data record and a theorist may speak of trajectories in a phase space. In order to not obscure the core concepts, more abstract orderings or partial orderings of primitive events are not discussed but the careful reader will be able to find appropriate launch points off the main storyline for application specific digressions.

The initial connections are made using the Birkhoff version of the Ergodic Theorem but before implications of that theorem are spun off some preparatory review of equilibrium thermodynamics and necessary conventions for reference frames are introduced.

Further fundamental connections are made once the Principle of Matched Invariants is introduced. This principle, and its implications, nail down the temperature field in time up to an ambiguity in the sense of orientation and a choice of scale. The orientation ambiguity is resolved insisting on the notion of an absolute zero and an appeal to causality. The notion of heat and work are introduced along with the first law of thermodynamics.

Warning: The second law is not introduced as a foundational principle but instead, as an example of a nonstandard application of the foregoing first law apparatus (and as a way to enter a discussion of the second law in a concrete setting) the thermodynamic interpretation of a simple closed queueing model is presented. It is argued that the context of that discussion allows for the least upper bound of the heating rate to be specifically identified.

2 Definitions and Conventions

In classical equilibrium thermodynamics it is supposed that the trajectory of the total system moves under the influence of its Hamiltonian and that at all times the trajectory lies on a surface of constant energy, i.e. that total system energy is conserved.

Of special interest in this work is the situation where only a subset of the total system is observed directly. Energies resident in the modes of the observed subsystem at a particular time are considered to be fluctuations derived from the total system as it moves on the constant energy surface.

In this case, the total system Hamiltonian is considered to be the sum of a Hamiltonian which governs the motion of the bath (the total system minus the subsystem) and a second Hamiltonian which governs the motion of the subsystem itself. Concerns about the lack of an interaction Hamiltonian are not relevant to the present purpose.

In the event that the energy of the total system is changed, the trajectories of the total system leave the former surface (at the old constant energy) and inhabit a new surface (at the new total energy). These energy surfaces are indexed by temperature. In what follows the raising or lowering of the total system trajectory from one energy surface to another is taken to be, by convention, a temperature change.

Mathematically, the same effect of raising or lowering the surface on which the total system energy resides could be achieved say, by addition of a reference energy to the subsystem Hamiltonian. In this work, by convention, once a reference energy is selected further uniform change of the subsystem state energies is interpreted as a temperature change of the total system.

From the point of view of the subsystem, an arbitrary reassignment of state energies may always be uniquely decomposed into changes about the old reference point which leave it unchanged (herein termed zero-sum changes), followed by a uniform shift in the reference point (interpreted as a temperature change in the bath). The zero sum changes will be interpreted as changes to the subsystem Hamiltonian.

For the sake of simplicity, consider a finite system with finitely many possible energies.¹ Let the set of states available to the subsystem be denoted by

$$\mathbf{v} = \{v(1), v(2), \dots, v(N)\} \quad (1)$$

A *data record* consists of a finitely long sequence of states visited along with the length of time each visit in the sequence lasted. For any given data record there is a rare state. That is, the one state that the system spent the least

¹As an assurance for the reader please note that the conventions adopted in this section leave us with subsystems and subsystem Hamiltonians the properties of which are consistent with and are in fact shared by the popular Ising Model for a bounded portion of a lattice magnet in finite dimensions. Further, a projection of the total dynamics onto N states may be accomplished in a variety of ways. Presentation of such a computation, at this point, would obscure the development of the fundamentals.

amount of discrete time in.² A data record may contain one, two or more visits to the rare state. The data record may be decomposed into cycles beginning and ending with visits to the rare state and the following cycle statistics may be collected:

the average number of discrete visits to each state during a data record averaged cycle,

$$\boldsymbol{\pi} = \{\pi_1, \pi_2, \dots, \pi_N\} \quad (2)$$

the average rate of a visit for each state during a data record averaged cycle,

$$\mathbf{q} = \{q_1, q_2, \dots, q_N\}. \quad (3)$$

That is, q_i^{-1} is the continuous time length of a typical visit to the i^{th} state.

The Carlson depth in this setting is the continuous time length of the characteristic cycle between visits to the rare state given by

$$CD = \frac{\pi_1}{q_1} + \frac{\pi_2}{q_2} + \dots + \frac{\pi_N}{q_N}. \quad (4)$$

All of the quantities introduced so far are, in principle, easily computed from a sufficiently detailed data record. On the other hand, of equal interest to the theoretically minded observer is the the Hamiltonian of the subsystem and the temperature of the bath it is connected to (by way of fluctuation exchanges). In what follows, it is supposed that energy and temperature have the same units, i.e. that the Boltzmann “ k ” has been absorbed into the temperature parameter. At this point the notions of energy and temperature are taken to be primitives but as the development proceeds that will begin to change.

To each state $v(i) \in \mathbf{v}$ let there be an energy assignment H_i . Introduce

$$\mathbf{H} = \{H_1, H_2, \dots, H_N\} \quad (5)$$

The assignments in (5) are taken to be real numbers with units of energy and serve as the Hamiltonian for the subsystem. The entire subsystem is assigned a single temperature value, denoted by the symbol θ . θ takes its numerical values in the positive real numbers. It carries units of energy.

The following constraint ensures that the changes made to the Hamiltonian do not include uniform additive shifts in reference point (which will expressed as temperature changes),

$$\Sigma H_k = 0.^3 \quad (6)$$

2.1 Two Great Measures and Ergodicity

While pursuing implications of the Birkhoff–Von Neumann quasi-ergodic hypothesis is one of the chief goals of this paper a detailed dissection of the argument is not. For the purposes of continuity in the storyline it is simply noted

²In case of a tie-pick your favorite!

³The fixed choice of energy reference. This state of affairs is implicit in the Ising model, for a familiar example.

that according to the Liouville Theorem the fraction of time spent in the neighborhood of a phase point along the trajectory is proportional to the volume of the neighborhood, which is preserved by the motion. That is, it is suggested that two measures are at play and that the observations contained in a data record using either language should be directly comparable.

The first measure is based on the (relative) amount of time spent in particular region of the phase space. The second is based on the (relative) volume of the region. As is well known, in the case of thermal equilibrium, the volume based measure takes on the form of Gibbs-Boltzmann fame in which the dependency on the energy of the region of phase space and temperature of the bath is made explicit.

In accord with these principles, in the context considered in this paper, two measures are taken to be directly comparable.

The first measure is the amount of time the observed system spent in a particular state $v(k) \in \mathbf{v}$ relative to the total length of the data record. In the terminology of equation(4)

$$\text{Prob}(v(k)) = \frac{\frac{\pi_k}{\mathbf{q}_k}}{\text{CD}}. \quad (7)$$

The second measure is the microcanonical one, i.e. the relative volume of the region in phase space,

$$\text{Prob}(v(k)) = \frac{e^{-\frac{H_k}{\theta}}}{Z} \quad (8)$$

where,

$$Z = e^{-\frac{H_1}{\theta}} + e^{-\frac{H_2}{\theta}} + \dots + e^{-\frac{H_N}{\theta}}. \quad (9)$$

A first easy consequence of (7), (8), and (6) is

$$H_k = \theta \log \left(\frac{\Pi}{x_k} \right) \quad (10)$$

where,

$$x_k = \frac{\pi_k}{\mathbf{q}_k} \quad k = 1, 2, \dots, N \quad (11)$$

$$\Pi = \left(x_1 x_2 \dots x_N \right)^{\frac{1}{N}} \quad (12)$$

and the x_k take values in the positive real numbers and carry dimensions of time.

Equation (10) is an inspiration. It suggests that, within the range of validity of the conventions and conditions adopted, more is contained in the experimentalist's data record than mere statistics. The path itself is described there and perhaps implicit in the time and frequency description of the path lies the energy and temperature description. If only θ were known as a function of the (x_1, x_2, \dots, x_N) equation (10) would deliver the state energies.

It is perhaps somewhat surprising at the outset, that there is so very little ambiguity in what the function that maps θ to (x_1, x_2, \dots, x_N) must be. In fact, figure 1 at the end of the next section, is a perspective of a constant temperature surface in time for a subsystem with three states, i.e. the case $N = 3$.⁴

The next section develops machinery to seek out surfaces of constant temperature in time. Before leaving this section, please note that a dilatation of the energy temperature space, i.e. the mapping

$$(\mathbf{H}; \theta) \rightarrow (\mathbf{H} + \epsilon \mathbf{H}; \theta + \epsilon \theta)$$

where ϵ is the real valued dilatation parameter, leaves the probabilities in (8) invariant.

Similarly, a dilatation of the time coordinates (x_1, x_2, \dots, x_N) from (11) leaves the probabilities described in (7) invariant. That is, probabilities are constant along rays in either space. A moments reflection reveals that dilatation is the only mapping that leaves the pointwise probabilities invariant.⁵

3 Matched Invariants Principle

A single experiment is performed and two observers are present and taking notes. The first observer creates a data record from which the quantities referenced in (2) and (3) may be computed. The second observer creates a data record in such a way that the quantities in (5) and θ are readily computed. The goal is to discover the method of observer number two.

The output of a single experiment then is two data points (one per observer): a single point in the (x_1, x_2, \dots, x_N) space and a single point in the $(H; \theta)$ space.

In the event that another experiment is performed and the observers repeat the activity of the previous paragraph, the data points generated are either both the same as the ones they produced as a result of the first experiment or else both are different. This is the essence of the principle—the two observers are using different languages to describe a *single* event. It is convenient to think that a series of experiments are under observation. The sequence of data points generated by an observer traces out a curve. There will be one curve in each space. It is assumed that the curves share a single, common parameterization. That is, that the two observers share the same clock.

The principle follows: in terms of probabilities, the two observers will continue to produce consistent results in the special case where the data points in their respective spaces have changed from the first experiment to the second but the probabilities have not. That is, if one observer experiences a dilatation so does the other.

⁴Constant temperature surfaces may be computed for arbitrary finite N but it is tough to produce the figure! Hence, $N = 3$.

⁵For example, a rotation may leave the total probability of a set unchanged (for example a cone symmetric about the axis of rotation) but the N probabilities of any single point in the set will not be invariant under the rotation.

Of course, if the observers are able to agree if dilatation has occurred they are also able to agree that it has not. In particular, in terms of differential displacements of the data points, the observers are able to decompose a displacement into a components parallel to the dilatation direction and perpendicular to it. Further, the observers are able to agree which component is which.

A good local set of coordinates for the observers consists of the dilatation direction (that's one dimension so far...) and any N-1 of the N probability gradients, ∇P_k , $k = 1, 2 \dots, N$. A concrete example of what these gradients are and how they are applied to compute constant temperature surfaces via the matched invariants principle will be developed in the next few subsections.

It is useful to note that, in either space, all probability gradients are perpendicular to the direction of dilatation.⁶ As a consequence of the matched invariants principle, the two observers can agree on the event that the computed probabilities change and that the associated trajectories in thier respective spaces are perpendicular to the dilatation direction at each point.⁷

Summary: The probabily invariant direction is the dilatation direction. In the setting of a system with N possible states, the N-1 dimensional space perp to the dilatation is spanned by any set of N-1 probability gradients.

3.1 Comparison of Trajectories Perpendicular to the Dilatation Direction

As was foretold, the ultimate purpose of this subsection is to apply the matched invariants principle and develop the machinery that will allow observer number one to compute constant θ surfaces in (x_1, x_2, \dots, x_N) space.

For the purposes of keeping those calculations straightforward, albeit at the cost of some clarity in the theoretical development, a specific reference frame is introduced and eventually a specific number of dimensions will be chosen. It is hoped that the symmetry of the result, displayed in the figure 1, will serve a posteriori to boost the level of theoretical clarity.

In what follows observer number one chooses coordinates (x_1, x_2, \dots, x_N) ⁸ and observer two chooses independent coordinates $(H_1, H_2, \dots, H_{N-1}, \theta)$.⁹

Local trajectories are decomposed into components along the probability gradients and along the dilatation direction. The form of these gradients is displayed next.

⁶Pointwise probabilities are invariant under dilatation

⁷If a trajectory may be expressed as a sequence of displacements each displacement perpendicular to the dilatation direction then the trajectory lies on the surface of a sphere. That is, the differential relation

$$\mathbf{x} \cdot d\mathbf{x} = 0 \tag{13}$$

defines the surface of the sphere.

⁸Recall equation (11)

⁹Recall equation (6).

On the observer one side, consider p_1 for example: ¹⁰

$$\nabla p_1 = \frac{1}{CD} \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} - \frac{p_1}{CD} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \quad (14)$$

Note that $\nabla p_1 \cdot \mathbf{x} = 0$.

Meanwhile, on the observer two side: ¹¹

$$\nabla p_1 = p_1 \begin{pmatrix} -\frac{1}{\theta} \\ 0 \\ \vdots \\ 0 \\ \frac{H_1}{\theta^2} \end{pmatrix} - p_1 \begin{pmatrix} \frac{p_N - p_1}{\theta} \\ \frac{p_N - p_2}{\theta} \\ \vdots \\ \frac{p_N - p_{N-1}}{\theta} \\ \frac{U}{\theta^2} \end{pmatrix} \quad (15)$$

Note that $\nabla p_1 \cdot (H; \theta) = 0$.

Beyond dilatation, another thing that observers can agree upon is the magnitude of changes in the state probabilities. ¹² In particular, probability changes that arise due to transitions in the plane perpendicular to the dilatation direction can be agreed upon. Recall that this space is spanned by any $N-1$ of the probability gradients.

Consider a specific example, the case where $N = 3$. A finite size step, $\Delta \mathbf{x}$, (suitable for use in a numerical scheme) perpendicular to the dilatation direction has the form

$$\Delta \mathbf{x} = \Delta_1 \frac{\nabla p_1}{\sqrt{\nabla p_1 \cdot \nabla p_1}} + \Delta_2 \frac{\nabla p_2}{\sqrt{\nabla p_2 \cdot \nabla p_2}} \quad (16)$$

where Δ_1 and Δ_2 are small numbers. That is, (16) is an experimentalist's approximation of the mathematician's differential. Once limits are taken, the change in probabilities incurred by the displacement (16) are given by:

$$dp_1 = \nabla p_1 \cdot d\mathbf{x} \quad (17)$$

$$dp_2 = \nabla p_2 \cdot d\mathbf{x} \quad (18)$$

Similar equations hold in the energy space. In the case where $N = 3$, the general displacement perpendicular to the direction of dilatation is lies in the space spanned by any two of the probability gradients in that space. In

¹⁰Recall equations (7) and (11). Derivatives have been taken with respect to the coordinates x_1, x_2, \dots, x_N .

¹¹Recall (8). Derivatives have been taken with respect to $H_1, H_2, \dots, H_{N-1}, \theta$.

¹²See the discussion surrounding ergodicity and the direct comparison of (7) and (8).

$(H_1, H_2, \dots, H_{N-1}, \theta)$ coordinates, observer number two's analog of equation (16) is a linear combination of those gradients

$$(\delta H, \delta \theta) = \delta_1 \frac{\nabla \mathbf{p}_1}{\sqrt{\nabla \mathbf{p}_1 \cdot \nabla \mathbf{p}_1}} + \delta_2 \frac{\nabla \mathbf{p}_2}{\sqrt{\nabla \mathbf{p}_2 \cdot \nabla \mathbf{p}_2}}. \quad (19)$$

The second observer's analog of (17) and (18) are

$$d\mathbf{p}_1 = \nabla \mathbf{p}_1 \cdot (dH, d\theta) \quad (20)$$

$$d\mathbf{p}_2 = \nabla \mathbf{p}_2 \cdot (dH, d\theta) \quad (21)$$

Observers agree on the probability changes seen so that:

$$d\mathbf{p}_1 = dp_1 \quad (22)$$

$$d\mathbf{p}_2 = dp_2 \quad (23)$$

Importantly, equations (22) and (23) provide a relation between the Δ 's from equation (16) and the δ 's from equation (19)

$$\begin{pmatrix} \delta_1 \\ \delta_2 \end{pmatrix} = \begin{pmatrix} \|\nabla \mathbf{p}_1\| & \frac{\nabla \mathbf{p}_1 \cdot \nabla \mathbf{p}_2}{\|\nabla \mathbf{p}_2\|} \\ \frac{\nabla \mathbf{p}_2 \cdot \nabla \mathbf{p}_1}{\|\nabla \mathbf{p}_1\|} & \|\nabla \mathbf{p}_2\| \end{pmatrix}^{-1} \begin{pmatrix} dp_1 \\ dp_2 \end{pmatrix}. \quad (24)$$

Equation (24) is the relation that observer one was looking for. If observer two supplies the δ 's observer one can translate them into Δ 's using (24), (22), (23), (17), (18) and (16). That is, changes in θ can be translated into changes in the time coordinates.

A consequence of (22) and (23) under the agreement that the observers share the same clock is

$$\dot{\mathbf{p}}_1 = \dot{p}_1 \quad (25)$$

$$\dot{\mathbf{p}}_2 = \dot{p}_2 \quad (26)$$

where the dot denotes differentiation with respect to the single, common curve parameter.

3.2 Consequence of Matched Invariants Principle

Another consequence of the matched invariants principle is that, as one moves perpendicularly to the dilatation direction from one point to the next along

the surface of a sphere in the (x_1, x_2, \dots, x_N) space, the ratio of temperature changes along the ray (the dilatation of temperature) remains constant.¹³

Further aspects of the example, $N = 3$, from the previous section are developed in this subsection. Consider two nearby points along the same ray, $r_{initial}$ in (x_1, x_2, x_3) space: $A = \{x_1, x_2, x_3\}$ and $A' = \{x_1 + \alpha x_1, x_2 + \alpha x_2, x_3 + \alpha x_3\}$ where $\alpha \ll CD$. Since the two points are on the same ray they generate the same probabilities (as do their images in $(\mathbf{H}; \theta)$ space) and in particular

$$\frac{H_k - U}{\theta}(A) = \frac{H'_k - U'}{\theta'}(A') \quad (27)$$

Suppose points A and A' on ray $r_{initial}$ undergo a small displacement $A \rightarrow B$ and $A' \rightarrow B'$ perpendicular to $r_{initial}$ (the direction of dilatation of the two points). Further suppose that points were displaced in such a way that the displaced points B and B' both lie on a ray, r_{final} .

Denote the temperature at A by θ and at A' by θ' . The temperature at B is given according to equations (19) and (15) by

$$\theta + \left[p_1 \frac{H_1 - U}{\theta} \right] \frac{1}{\theta} \frac{\delta_1}{\|\nabla p_1\|} + \left[p_2 \frac{H_2 - U}{\theta} \right] \frac{1}{\theta} \frac{\delta_2}{\|\nabla p_2\|} \quad (28)$$

The quantities in square brackets above are invariant along the ray and thus are the same at B and at B' . The scaling of the probability gradients along the ray from point A to A' may be observed from (15), for example as follows

$$\nabla p_1 \Big|_A = \frac{\theta'}{\theta} \nabla p_1 \Big|_{A'} \quad (29)$$

The scaling of the δ_K is obtained from equation (24) and the requirement that both B and B' lie on r_{final} , i.e. that the probability changes incurred along path $A \rightarrow B$ are the same as those along $A' \rightarrow B'$. For example, in the case of the first coordinate,

$$\delta_1 \Big|_{A \rightarrow B} = \frac{\theta}{\theta'} \delta'_1 \Big|_{A' \rightarrow B'} \quad (30)$$

Thus the temperature at B' is obtained from equations (28), (29) and (30) is found to be

$$\frac{\theta'}{\theta} \left(\theta + \left[p_1 \frac{H_1 - U}{\theta} \right] \frac{1}{\theta} \frac{\delta_1}{\|\nabla p_1\|} + \left[p_2 \frac{H_2 - U}{\theta} \right] \frac{1}{\theta} \frac{\delta_2}{\|\nabla p_2\|} \right) \quad (31)$$

Comparison of (28) and (31) reveals that the original ratio of temperatures at points A and A' on ray $r_{initial}$ is maintained by the motion $A \rightarrow B$ and $A' \rightarrow B'$ described above.

¹³The discussion which follows keeps the matched invariants principle to the fore. A simpler geometrical demonstration (obscuring the notion of observation of probabilities) goes as follows. Let two points on the θ -axis be labelled θ and θ' . Consider a rigid rotation in the $(H_1, H_2, \dots, H_{N-1}, \theta)$ space (L2 moduli of the original line segments on the theta axis maintained). The temperature at the rotated images are easily obtained by vector dot product with the theta axis. In the ratio the cosines disappear and the original ratio of the L2 moduli is maintained.

3.3 The Sense of Direction and Choice of Scale of the Theta to Centerline Map

Observer Two reports that along the θ axis in $(H_1, H_2, \dots, H_{N-1}, \theta)$ space the probabilities in (8) are uniform. Observer one reports that the same is true of the *centerline* axis, i.e. ray from the origin containing the $\{1, 1, \dots, 1\}$ vector, in (x_1, x_2, \dots, x_N) space. This simple observation identifies the image of the theta axis in the (x_1, x_2, \dots, x_N) space as the centerline.

Taking into account the results of the last two subsections, it is clear that knowing the behaviour of θ along the centerline allows Observer one to determine the θ field in (x_1, x_2, \dots, x_N) space completely.

Recall, that an algorithm has been prescribed which gives the evolution of θ along a spherical surface in the (x_1, x_2, \dots, x_N) space given the value of θ at the intersection of the surface with the centerline.

Once the θ values on a single spherical surface are obtained the rest of the field is determined via the preservation of θ dilatation property discussed in the previous subsection. Take the mapping of the θ axis to the centerline as the reference.

So what can be said about the centerline map? Important features of any continuous, one to one, and onto map between one-dimensional spaces include the sense of orientation (as one moves toward infinity along the centerline in (x_1, x_2, \dots, x_N) space is θ going to infinity or is θ moving to zero?) and for a given orientation, a choice of scale, i.e. the local stretching or shrinking of the map.

For example, the identity map $\theta(\text{CD}) = \text{CD}$ is a choice of temperature scale oriented such that theta goes to infinity as one moves out to infinity along the centerline. A simple inversion $\theta(\text{CD}) = \frac{1}{\text{CD}}$ is a choice of scale that takes theta to zero as one moves out to infinity along the centerline.

Note that the sense of direction of the map may be obtained form the following thought experiment: An experiment is conducted in a laboratory frame that produces a set of set changes in time-a data flow. One might think of this as a sort of information “velocity”, the rate at which an observer becomes aware that a state change has taken place. An observer in the laboratory frame measures the Carlson depth of the data flow.¹⁴

Now a second observer, moving at a constant “velocity” (with respect to the laboratory frame) forward into the data flow, sees exactly the same probabilities of events as the laboratory frame observer but witnesses the time inbetween visits to the rare state to pass by more quickly than the observer in the lab frame. In fact, the observer may move forward at arbitrarily large constant “velocity” and witness, the same sequence of ordered events occurring with the same probability as the laboratory frame observer but the Carlson depth shrinks to zero as the observer’s speed relative to the lab frame tends to infinity.

A third observer, moving more slowly than the observer in the laboratory frame, sees the data pass by more slowly than the lab observer. But, impor-

¹⁴Recall (4).

Surface of Constant Temperature in Time for the Three State System

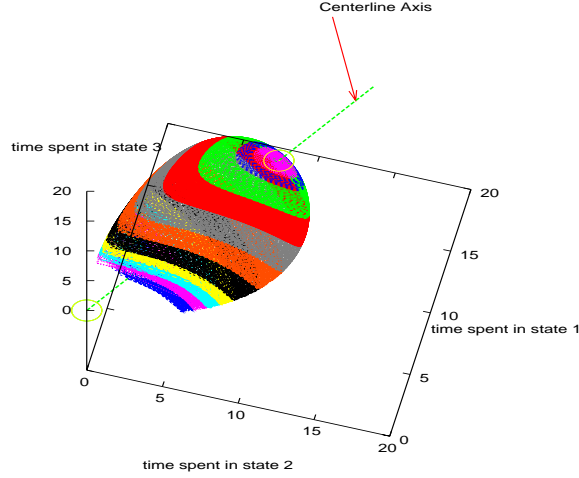


Figure 1: Isothermal Surface Drawn in Space of Statewise Contributions to Fundamental System Period for a Three State System

tantly, this decrease in “velocity” relative to the lab observer may not increase without bound. A point is reach when the travelling observer is moving away from the data at the same rate at which the data is moving toward her at which point: nothing changes. Identify this notion of total absence of change of the state of the system with the notion of absolute zero.

Hence we adopt the convention, consistent with the principle of casuality, that as the temperature is decreased to zero the recurrence time of the system is observed to increase and conversely.

This convention prescribes the sense of orientation of the map. It does not suggest a choice of scale. In fact, one conjectures that given many reasonable choices of scale there is some one-dimensional parameterized family of accelerating frames of observation that would produce results consistent with it. Analysis of those structures is not considered here.¹⁵

In the figure, a θ to centerline mapping $\theta(CD) = \frac{A}{CD}$, where A is a positive real constant, was taken as the choice of scale along the centerline. Note that the centerline axis is perpendicular to the surface at their intersection. Local to the centerline axis, the system period fixes the temperature (within a choice of scale). The reader may have their own favorite choice of temperature scale to which the Matched Invariants Principle may then be applied to generate the

¹⁵The author is indebted to S. Huntsman for pointing out the the analogy between the proceeding arguments and the Unruh-Davies Effect.

temperature field from which surfaces of constant θ (consistent with that choice of scale) may be isolated.

4 Application of the Foregoing to Closed Queueing System

In the previous sections, particular characteristics of the experiment generating the observed dynamics were never explicitly stated. The subject never came up. As a simple example of an application of the foregoing to a non-standard system, in this section, some thermodynamical aspects associated with the dynamics of a closed queueing network are derived.

Necessary fundamentals from elementary queueing theory and elementary thermodynamics are introduced, as required, along the way. The following queue construction is standard.¹⁶ Connections with the "Stosszahlansatz" may be found in work of Kac, Uhlenbeck and Siegert.¹⁷

Recall that a closed queueing system consists of N buckets and M balls. Traditionally the N buckets represent N servers say at the office of some government bureaucracy and the M balls are clients waiting to be served. That is, they wait in line to get to the counter at which time they are told they are in the wrong line and need to go to a different counter, hence closed.

At any moment in time an observer might see m_1 people at counter 1 (that is, m_1 balls in bucket 1) and m_2 balls in bucket 2 etc. The list of bucket occupancies observed, denoted by (m_1, m_2, \dots, m_N) , determines the instantaneous state of the system. An instantaneous state of the system will herein be referred to as a *configuration*. Let \mathbf{v} denote the set, indexed by the natural numbers, of all possible system configurations.

When the queue is observed in action, the list of configurations it visits in time (a list of lists indexed by time) forms the experimental record. It is the trajectory of the system as it moves through its state space.

Once a trajectory is in hand the statistics in (2), (3) and (11) may be collected. Further, it is known from the previous sections that there is only one way, consistent with the Matched Invariants Principle and the observers choice of temperature scale, to define a temperature field in (x_1, x_2, \dots, x_N) space where the computed statistics of the trajectory reside. By way of (10), the vector field of energies is generated next.

In the context of a specific system, like the present example, one can go further. It makes sense to look for work and heat.

Recall from elementary thermodynamics that the macroscopic observable energy is defined by

$$U = \mathbf{p} \cdot \mathbf{H} \quad (32)$$

¹⁶See for example, Kleinrock, L. *Queueing Systems*, Wiley, New York, 1975.

¹⁷See for example, A.J Siegert, *On the Approach to Statistical Equilibrium*, The Physical Review, v76, 1949.

where \mathbf{p} is given by (8) and \mathbf{H} by (5).

Take a derivative with respect to time to obtain

$$\dot{U} = \dot{\mathbf{p}} \cdot \mathbf{H} + \mathbf{p} \cdot \dot{\mathbf{H}}. \quad (33)$$

In the equilibrium setting, the RHS of (33) decomposes the rate of energy change into work rate and heat rate respectively.

That is to say the work rate is given by

$$\dot{W} = \mathbf{p} \cdot \dot{\mathbf{H}} \quad (34)$$

and the heating rate by

$$\dot{Q} = \dot{\mathbf{p}} \cdot \mathbf{H} \quad (35)$$

4.1 Compute $\mathbf{p}\dot{\mathbf{H}}$

Now the two vectors appearing in the dot product in the RHS of (34) are elements of a high-dimensional space (the cardinality of ν) while the work rate itself is a single scalar quantity. So in switching from the RHS to the LHS in (34) one also switches levels of description and goes from too much information to perhaps not enough. Thermodynamic tradition insists on the introduction of an alternative, a middle ground between information overload and ignorance.

What is required are two low dimensional vectors (low in comparison to the number of microscopic states ν represents) that contain sufficient information to characterize the observed trajectory and are equivalent to \mathbf{p} and $\dot{\mathbf{H}}$ in the sense that the inner product is the same in both sets of descriptions of the dynamics. Famous examples of such conjugate pairs are the pressure and rate of volume change in a gas and the average magnetization and applied field change in the case of a lattice magnet.

A good starting point is simply to write out exactly what the high-dimensional form of the work rate looks like.

Recall from (10)

$$H_{\cdot} = \theta \log \left(\frac{\Pi}{x_{\cdot}} \right) \quad (36)$$

where,

$$\Pi = \left(x_1 x_2 \cdots x_N \right)^{\frac{1}{N}}. \quad (37)$$

Equivalently,

$$H_{\cdot} = \theta \log \left(\frac{\mathfrak{J}}{p_{\cdot}} \right) \quad (38)$$

where,

$$\mathfrak{J} = \left(p_1 p_2 \cdots p_N \right)^{\frac{1}{N}}. \quad (39)$$

Therefore

$$\dot{H} = \dot{\theta} \log \left(\frac{\dot{\mathbf{J}}}{p} \right) + \theta \left(\frac{\dot{\mathbf{J}}}{\dot{\mathbf{J}}} - \frac{\dot{p}}{p} \right) \quad (40)$$

and so

$$\mathbf{p} \cdot \dot{\mathbf{H}} = \dot{\theta} \log \left(\frac{\dot{\mathbf{J}}}{\Lambda} \right) + \theta \left(\frac{\dot{\mathbf{J}}}{\dot{\mathbf{J}}} \right) \quad (41)$$

with

$$\Lambda = \left(p_1^{p_1} p_2^{p_2} \cdots p_N^{p_N} \right). \quad (42)$$

4.2 In Particular for the Closed Queue

The goal is to obtain a form of the work rate suitable for the closed queueing system. The calculations involved are simple but some further details about the construction of the queue are necessary before system specific calculations can begin.

A closed queue of M servers is constructed as a Markov process by characterizing the holding times of the servers, the interaction among the servers and the state space of the queue.

The characteristic times of the M servers are the rates in the exponential distribution that characterizes a particular servers processing time. Routing from one server to another is governed by an $M \times M$ matrix of transition probabilities, herein called the routing table. A basic transition occurs as follows: at the completion of a service time the server looks to the routing table for instruction. The length of the service is at the discretion of the server. The location of the client's next service is decided by the router.

It is well known that such a transition matrix admits an eigenvector with all positive coefficients. Without loss of generality take the minimum component of the eigenvector to have value 1 (the rare state gets visited once).

If m is the total number of clients in the system then the states of the queueing network are all M -long sequences of non-negative integers (zero is ok) that sum to m . As is well known, that number is given by

$$N = \binom{M + m - 1}{m} \quad (43)$$

In summary then, the equilibrium distribution of the closed queueing network is given by specifying the parameters for the exponentially distributed service times

$$\mathbf{q} = \{(q_1, q_2, \dots, q_M) : q_i \in \mathbf{R}^+\}. \quad (44)$$

The eigenvector, with eigenvalue 1, of the $M \times M$ matrix of probabilities (the routing table)

$$\pi = \{(\pi_1, \pi_2, \dots, \pi_M) : \pi_i \in [1, \infty) \text{ and } \pi_{rare} = 1\} \quad (45)$$

and the state space

$$\mathbf{v} = \{(v_1, v_2, \dots, v_M) : v_i \in \mathbf{Z}^+; v_1 + v_2 + \dots + v_M = m\}. \quad (46)$$

The equilibrium distribution for a closed queue is given by

$$\mathbf{Prob}(\alpha_1, \alpha_2, \dots, \alpha_M) = \frac{\left(\frac{\pi_1}{q_1}\right)^{\alpha_1} \left(\frac{\pi_2}{q_2}\right)^{\alpha_2} \dots \left(\frac{\pi_M}{q_M}\right)^{\alpha_M}}{\sum_{\mathbf{v}} \left(\frac{\pi_1}{q_1}\right)^{v_1} \left(\frac{\pi_2}{q_2}\right)^{v_2} \dots \left(\frac{\pi_M}{q_M}\right)^{v_M}}. \quad (47)$$

In this setting, the quantity \mathfrak{J} from (39) takes a particularly pleasing form

$$\mathfrak{J} = \frac{\left[\frac{\pi_1}{q_1} \frac{\pi_2}{q_2} \dots \frac{\pi_M}{q_M}\right]^{\frac{\alpha}{N}}}{\sum_{\mathbf{v}} \left(\frac{\pi_1}{q_1}\right)^{v_1} \left(\frac{\pi_2}{q_2}\right)^{v_2} \dots \left(\frac{\pi_M}{q_M}\right)^{v_M}} \quad (48)$$

where

$$\alpha = \sum_{k=0}^{m-1} (m-k) \binom{(M-1)+k-1}{(M-1)-1}. \quad (49)$$

Note that

$$\frac{\alpha}{N} = \frac{m}{M}. \quad (50)$$

The heart of the right hand side of (34) for the queue involves the particular expression

$$\frac{\mathfrak{J}}{\mathfrak{J}} = \frac{\left[\frac{\pi_1}{q_1} \frac{\pi_2}{q_2} \dots \frac{\pi_M}{q_M}\right]^{\frac{\alpha}{N}}}{\left[\frac{\pi_1}{q_1} \frac{\pi_2}{q_2} \dots \frac{\pi_M}{q_M}\right]^{\frac{\alpha}{N}}} - \frac{\left[\sum_{\mathbf{v}} \left(\frac{\pi_1}{q_1}\right)^{v_1} \left(\frac{\pi_2}{q_2}\right)^{v_2} \dots \left(\frac{\pi_M}{q_M}\right)^{v_M}\right]}{\left[\sum_{\mathbf{v}} \left(\frac{\pi_1}{q_1}\right)^{v_1} \left(\frac{\pi_2}{q_2}\right)^{v_2} \dots \left(\frac{\pi_M}{q_M}\right)^{v_M}\right]}. \quad (51)$$

After straightforward calculation this simplifies to

$$\frac{\mathfrak{J}}{\mathfrak{J}} = \frac{\alpha}{N} \left(\frac{\left[\frac{\pi_1}{q_1}\right]}{\frac{\pi_1}{q_1}} + \frac{\left[\frac{\pi_2}{q_2}\right]}{\frac{\pi_2}{q_2}} + \dots + \frac{\left[\frac{\pi_M}{q_M}\right]}{\frac{\pi_M}{q_M}} \right) - \left(\frac{\langle v_1 \rangle \left[\frac{\pi_1}{q_1}\right]}{\frac{\pi_1}{q_1}} + \frac{\langle v_2 \rangle \left[\frac{\pi_2}{q_2}\right]}{\frac{\pi_2}{q_2}} + \dots + \frac{\langle v_M \rangle \left[\frac{\pi_M}{q_M}\right]}{\frac{\pi_M}{q_M}} \right), \quad (52)$$

where the angle brackets denote the average is taken over the set (46) with respect to measure (47).

First of all, note that the description of the dynamics appearing on the RHS of (52) is low dimensional. Recall that M is the number of buckets and compare this with (43). Equally important, the pieces comprising the right hand side of (52) are easily recognizable.

Let Υ denote the average state of the system over an observation period,

$$\Upsilon = \mathbf{p} \cdot \mathbf{v} \quad (53)$$

that is, the average ball count per bucket.

Let $\boldsymbol{\eta}$ contain the performance information for each the M servers in the form of M ratios: average number of customers assigned to that server per characteristic cycle scaled by the servers characteristic rate

$$\boldsymbol{\eta} = \left\{ \frac{\pi_1}{q_1}, \frac{\pi_2}{q_2}, \dots, \frac{\pi_M}{q_M} \right\}. \quad (54)$$

In terms of these quantities the workrate takes the form

$$\dot{W} = \frac{\dot{\theta}}{\theta} U + \left(\frac{\alpha}{N} \mathbf{1} - \Upsilon \right) \cdot \frac{\dot{\boldsymbol{\eta}}}{\boldsymbol{\eta}}. \quad (55)$$

In the event that the work takes place at constant temperature we have simply

$$\dot{W} = \left(\frac{\alpha}{N} \mathbf{1} - \Upsilon \right) \cdot \frac{\dot{\boldsymbol{\eta}}}{\boldsymbol{\eta}} \quad (56)$$

The macroscopic work rate in the RHS of (56) does all the things we need it to. The number of dimensions of the vectors involved have been greatly reduced and the M-dimensional vectors obtained represent meaningful coarse characteristics of the system. The dot product, i.e the scalar value of the work rate, has been preserved. The first law of thermodynamics is observed by definition. What about the second law?

The second law question will be the subject of the next subsection. Before getting there two additional famous thermodynamic quantities are presented for this system. The calculations are similar to the example just given and will be omitted.

The Helmholtz Free Energy:

$$F = -\log \left(\sum_{\gamma \in \mathbf{v}} \left(\frac{\pi_1}{q_1} \right)^{\gamma_1 - \frac{\alpha}{N}} \left(\frac{\pi_2}{q_2} \right)^{\gamma_2 - \frac{\alpha}{N}} \dots \left(\frac{\pi_M}{q_M} \right)^{\gamma_M - \frac{\alpha}{N}} \right) \quad (57)$$

The Internal Energy:

$$U = \theta \left\langle \log \left(\left(\frac{\pi_1}{q_1} \right)^{v_1 - \frac{\alpha}{N}} \left(\frac{\pi_2}{q_2} \right)^{v_2 - \frac{\alpha}{N}} \dots \left(\frac{\pi_M}{q_M} \right)^{v_M - \frac{\alpha}{N}} \right) \right\rangle \quad (58)$$

where the angle brackets denote the average is taken over the set (46) with respect to measure (47).

4.3 2nd Law for the Closed Queue

The purpose of last subsection was to gather together and present a few famous thermodynamical highlights of this queue system.

Among these highlights however there is one quantity that is more than just a mere calculation. This quantity is the the least upper bound for the heating rate of the queue and is a specific example of what is considered, in its abstract form, to be at the very heart of the Second Law.

If a least upper bound for the system can be identified concretely then it does not need a Law to justify its existence. It is simply a matter of proving that an inequality is sharp.

In this particular system, the existence of a least upper bound for the heating rate is very nearly obvious. The proof is simply a matter of making the right definitions. Perhaps the following heuristic argument for sharpness will suffice. Consider that there are two probabilities at play: (7) and (47).

In equilibrium¹⁸, the two measures are the same, equal. But what happens when the queue transitions to a new equilibrium? Suppose, for example, that the routing table is changed very slowly in such a way that no work is performed¹⁹ and that the energy is increased.

Since the routing table has changed, its eigenvector, (45) may also change and so also the probabilities given by description (47). The probabilities given in (7) will eventually converge to the new (47).

An observer watching the routing table needs to see each altered element of the $M \times M$ table route quite a few customers before being satisfied that the new table values have been empirically discovered and the new equilibrium achieved.

However, an observer watching the state space \mathbf{v} needs to see each of the N states, recall (43), transition many times before being satisfied that the probabilities of each microscopic state given in (7) have been empirically discovered.

Note that a microstate transition cannot occur without a routing table action, i.e. the two “step” in time at exactly the same scale but that, in practice, the number N dwarfs the number M squared.

In this situation, it is not unreasonable to suppose that the observer of the routing table will become empirically satisfied that the table entries have converged to their new values and that the new energy level has been attained long before the \mathbf{v} observer sees each microstate in the state space visited even once, let alone visited sufficiently many times that there is some empirical sense of convergence.²⁰

Still one might imagine, along with Carnot, a series of very small perturbations of the routing table with very long periods of time inbetween such that the two descriptions (7) and (47) are very nearly equal at all times.

The heating upper bound proposed for this system is given by

$$\dot{Q}^+ = \theta \frac{\dot{\eta}}{\eta} \cdot [\langle v(\cdot) \rceil \rangle - \langle v(\cdot) \rangle \langle \rceil \rangle] \quad (59)$$

where the angle brackets denote the average is taken over the set (46) with

¹⁸Equilibrium in this context is taken to mean that the routing table values and service rates are constant in time,

¹⁹The work rate is identically zero throughout the transition.

²⁰In short, the “covering time of the routing table” is much, much smaller than the covering time of the state space: the steps of the covering walks occur at identical rates (in fact they step at exactly the same time, every time), the graphs are comparable (the routing table graph is approximately a quotient space of the set of edges of the \mathbf{v} graph, mod out by “direction”) but obviously one, the \mathbf{v} graph, is much much bigger.

respect to measure (47),

$$\Upsilon = \log \left(\left(\frac{\pi_1}{q_1} \right)^{\frac{\pi}{N} - v_1} \left(\frac{\pi_2}{q_2} \right)^{\frac{\pi}{N} - v_2} \dots \left(\frac{\pi_M}{q_M} \right)^{\frac{\pi}{N} - v_M} \right) \quad (60)$$

and

$$v(\cdot) = \{v_1, v_2, \dots, v_M\} \quad (61)$$

denotes an element of the set \mathbf{v} from (46).²¹

The derivation of (59) is of the same type as the derivation of the work rate presented above except that the starting point is (35) instead of (34).

The heating rate stands unadorned

$$\dot{Q} = \dot{p} \cdot \mathbf{H} \quad (62)$$

where recall,

$$H_k = \theta \log \left(\frac{\Pi}{x_k} \right), \quad (63)$$

and

$$x_k = \frac{\pi_k}{\mathbf{q}_k}, \quad k = 1, 2, \dots, N. \quad (64)$$

The π 's and q 's are obtained by observing the trajectory on v . This definition of heating rate is consistent with the usual notion of heat as a microscopic quantity.

Note that when the system is at equilibrium (7) and (8) are directly comparable and \dot{Q} is the heating rate per (25), (26) and (35).

²¹Of course, $\langle v(\cdot) \rangle$ is simply Υ from (53).